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# Variational Calculations for Liquid Na-Cs Alloy

# II. The Heat Capacity at Constant Pressure

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**Abstract**

The heat capacity at constant pressure of the Na-Cs equiatomic liquid alloy at $T$=373K is calculated by the variational method with hard-sphere reference system. It is found that the Krasco-Gurskiy model pseudopotential with the Geldart-Vosko exchange-correlation function gives a slightly better agreement with the experiment than the local Animalu-Heine model pseudopotential with the Toigo-Woodruff exchange-correlation function.

**Keywords:** Variational method, pseudopotential theory, liquid binary metal alloy, heat capacity at constant pressure

The heat capacity at constant pressure, $c_P$, is determined as follows:

$$c_P = T\left(\partial\Omega / \partial T\right)_P \quad , \tag{1}$$

where $\Omega$ is the mean atomic volume, $P$ – pressure, $T$ – temperature.

In present study, Eq. (1) is calculated numerically from $\Omega$ obtained by the variational method (described in paper I [1]) by using the following condition:

$$\left(\partial F / \partial\Omega\right)_{T,\sigma_{ij}} = 0 \quad , \tag{2}$$

where $F$ is the Helmholtz free energy, $\sigma_{ij}$ – partial hard-sphere diameter, $i,j$=1,2.

Two combinations of the pseudopotential model with the exchange-correlation function (ECF) are used: 1) the local Animalu-Heine (AH) [2] model pseudopotential (MP) with the Toigo-Woodruff (TW) [3] ECF; 2) the Krasco-Gurskiy (KG) [4] MP with the Geldart-Vosko (GV) [5] ECF. The local AH pseudopotential form-factor was presented in paper I. An analogous function

for the KG MP is written as follows:

$$\omega_i^{\mathrm{KG}}(q) = -\left(4\pi z / \Omega q^2\right)\left\{(2a_i - 1)q^2 r_{ci}^2 - 1\right\} \Big/ \left(1 + q^2 r_{ci}^2\right)^2 \Big) \ , \qquad (3)$$

where $z$ is the mean alloy valence, $a_i$ and $r_{ci}$ – $i$-th component parameters taken the same as for the corresponding pure metal.

**Table 1**. Values of pseudopotential parameters [3] used as input data

| | $A$ (a.u.) | $R_{\mathrm{M}}$ (a.u.) | $a$ (a.u.) | $r_{\mathrm{c}}$ (a.u.) |
|---|---|---|---|---|
| Na | -0.1958 | 2.1148 | 0.4898 | 3.242 |
| Cs | -0.1838 | 3.8677 | 0.8440 | 2.586 |

**Table 2**. Calculated heat capacity at constant pressure of the Na-Cs equiatomic liquid alloy at $T$=373K in comparison with the experiment [6]

| | AH-TW | KG-GV | Exp. |
|---|---|---|---|
| $c_P / k_{\mathrm{B}}$ | 4.30 | 4.21 | 3.90 |

As it can be seen, the difference with experiment not more than 10 percent in both calculations, but the KG-GV combination gives a slightly better agreement.

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